

Exploring scalar quantum walks on Cayley graphs

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A quantum walk, *i.e.*, the quantum evolution of a particle on a graph, is termed *scalar* if the internal space of the moving particle (often called the coin) has a dimension one. Here, we study the existence of scalar quantum walks on Cayley graphs, which are built from the generators of a group. After deriving a necessary condition on these generators for the existence of a scalar quantum walk, we present a general method to express the evolution operator of the walk, assuming homogeneity of the evolution. We use this necessary condition and the subsequent constructive method to investigate the existence of scalar quantum walks on Cayley graphs of various groups presented with two or three generators. In this restricted framework, we classify all groups – in terms of relations between their generators – that admit scalar quantum walks, and we also derive the form of the most general evolution operator. Finally, we point out some interesting special cases, and extend our study to a few examples of Cayley graphs built with more than three generators.

I. INTRODUCTION

Within the traditional (discrete-time) model of quantum computation, there exist several definitions for a quantum walk on a given graph G over a set of vertices X . In general terms, a quantum walk simulates the evolution of a particle on the graph with some unitary operator as an evolution operator. The most studied model, the “coined model”, defines the evolution operator as the product of two operators. One is a block diagonal operator which acts non-trivially only on some internal space of the particle, termed the “coin”. The other operator is a permutation which moves the particle along the edges of the graph. In that model, the most common definition, which has been used for constructing existing quantum walk algorithms, is the one given by Aharonov *et al.* in [1]. Within this definition, the condition for the existence of such operators is that the graph G is an oriented d -regular graph and that it is possible to “label each directed edge with a number between one and d such that for each possible label a , the directed edges labeled a form a permutation”.

Kendon gave another definition [2], which is valid for non oriented graphs where the coin is of dimension $|X|$, the number of vertices. In fact both definitions can be seen as particular cases of the definition given by Montanaro in [3]. Following the latter work, a necessary and sufficient condition to define a coined quantum walk is *reversibility*. When a graph is reversible, it has a certain number of cycles which may be used to define a coined quantum walk. The idea is that each cycle is associated to a basis state of the internal space, using the fact that cycles that do not have a vertex in common can be associated to the same basis state. The definition of Aharonov *et al.* requires the graph to be d -regular (and therefore reversible), with exactly d groups of disjoint cycles including all edges of the graph. Kendon’s definition also requires a reversible graph, and in this case the cycles used are determined by each directed edge and the corresponding edge with opposite direction. Therefore, reversibility and the number of cycles in the graph may be used to classify the different possible definitions in a two operator (coined-shift) model of quantum walks.

If we do not restrict to the coined model (that is, we do not assume that the evolution operator factorizes into two operators), no sufficient condition is known for the existence of a unitary evolution operator on a given graph. Presently, only some necessary conditions are known, one of them being reversibility. In [4], quantum walks with one operator and with internal space (coin) are explored. It is shown how the existence of such walks is related to the properties of the graph and some examples are given. If the model has an internal space of dimension one, the one-operator model corresponds to the definition used in [5] and quantum walks become in this case equivalent to quantum cellular automata as defined by Meyer in [6]. Here, we will call this model (one operator and a one-dimensional internal space) a *scalar quantum walk*.

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In [5], Severini gave a necessary condition for the existence of a scalar quantum walk on a graph, that he called *strong quadrangularity*. The strong quadrangularity implies another condition called *quadrangularity*. Together with specularity, strong quadrangularity becomes sufficient for the existence of a unitary evolution on the graph. In general terms, a graph is called *specular* if any two vertices are connected by outgoing edges to the same set of vertex or do not have any common first neighbor, the same being required for the ingoing edges. Specularity is equivalent to the condition that the operator may be expressed as the product of a permutation matrix and a block diagonal matrix, which means that the evolution operator takes in this case the form of a coined evolution operator on a smaller graph [7].

In this paper, we will address the general question of determining on which Cayley graphs a homogeneous scalar quantum walk can be defined. First, there is an obvious interest in this question from the point of view of quantum algorithmics. Indeed, the answer will help defining gates over graphs, which could then be combined to construct quantum algorithms. Moreover, algorithms based on scalar quantum walks in the circuit model can also be compared in a more natural way to quantum walks in continuous-time models of quantum computation, such as adiabatic quantum computation. Apart from these algorithmic applications, there are also true conceptual differences between scalar and coined quantum walks, which make them both interesting topics of studies on their own. In the classical case, note that random walks using an internal state space exhibit a memory effect, which makes their classical evolution non-Markovian [8] in contrast to random walks with no internal space. In the quantum case, the behavior of scalar quantum walks is a more direct consequence of a purely quantum effect, namely phase interference, since adding an internal space necessarily prevents interferences between paths. Finally, we observe that the efficiency of the algorithms using quantum walks varies with the dimension of the internal space without any obvious reason [9], so that it seems to be important to investigate both scalar and coined quantum walks to solve an algorithmic problem on a given search space.

To identify the Cayley graphs that accept a scalar quantum walk, we will first verify whether some necessary conditions are satisfied for various graphs. First, we know that all Cayley graphs are reversible. The other known conditions are quadrangularity and strong quadrangularity. While the condition of strong quadrangularity depends on the number of subsets of the vertex set of the graph, and thus requires an exponential time to be checked, the quadrangular condition depends on the number of pairs of vertices and may be checked in polynomial time. We will thus use quadrangularity as a necessary condition. This paper is organized as follows. In Section II, we will derive the quadrangular condition and adapt it to homogeneous quantum walks on Cayley graphs. In Section III, we will present a general method allowing us to determine whether a homogeneous scalar quantum walk exists on a given Cayley graph and, if so, to explicitly derive its evolution operator. In Section IV, we will apply the above necessary condition and constructive method in order to find new scalar quantum walks. We will consider a variety of Cayley graphs, built from two, three, and occasionally more than three generators.

II. CONDITIONS ON THE EXISTENCE OF SCALAR QUANTUM WALKS ON CAYLEY GRAPHS

A. Quadrangularity for general graphs

Let $G(X, E)$ be a graph with vertex set X and edge set E . A scalar quantum walk is a model of the evolution of a particle on the graph G . The state of the particle is described by a unit vector in the Hilbert space $H = \ell^2(X)$ and we will use the set of states $\{|x\rangle\}_{x \in X}$ as a basis for H . The evolution operator W is a unitary operator on H . The evolution of $|\psi_t\rangle$, the state describing the position of the particle at time t , is given by the following equation:

$$|\psi_t\rangle = W^t |\psi_0\rangle, \quad (1)$$

where $|\psi_0\rangle$ is a given initial state. We denote as $W_{x,y}$ the matrix elements $\langle x|W|y\rangle$. A necessary condition for the existence of a scalar quantum walk on a graph is called quadrangularity. It was first presented in [5], and can also be obtained as a consequence of the analysis presented in [4]. Let us recall it here.

Proposition 1. *Given a graph $G(X, E)$, if a scalar quantum walk on this graph exists then for each pair of different edges of the form (x, z) and (y, z) there exists another pair of different edges of the form (x, z') and (y, z') .*

Proof. The equation $W^\dagger W = \text{Id}_H$, where W^\dagger is the conjugate transpose of W and Id_H is the identity on H , is equivalent to the set of equations:

$$\begin{cases} \sum_{z \in X} \overline{W}_{z,x} W_{z,y} = 0 & \forall x, y \in X, x \neq y \\ \sum_{z \in X} \overline{W}_{z,x} W_{z,x} = 1 & \forall x \in X \end{cases} \quad (2)$$

And the matrix equation $WW^\dagger = \text{Id}_H$ is equivalent to

$$\begin{cases} \sum_{z \in X} W_{x,z} \overline{W}_{y,z} = 0 & \forall x, y \in X, x \neq y \\ \sum_{z \in X} W_{x,z} \overline{W}_{x,z} = 1 & \forall x \in X \end{cases} \quad (3)$$

where $\overline{\alpha}$ denotes the complex conjugate of α . Suppose that the sum in the first type of equation contains only one term for some couple (x, y) . Then, the only possibility for the condition to be satisfied is to have one of the two coefficients equal to zero. This is equivalent to modifying the graph, so that in this case, there is no scalar quantum walk for the original graph G . \square

This proposition can also be reformulated as follows:

Given a graph $G(X, E)$, if a scalar quantum walk on this graph exists then all consecutive edges in the graph with different orientations belong to at least one closed path of length four with alternating orientations.

B. Quadrangularity for Cayley graphs

A Cayley graph is a graph constructed using the relations of a group. Given a group Γ and a set Δ of elements generating the group (all elements in Γ may be obtained by multiplication of elements and inverse elements of the generating set), the Cayley graph $C_\Delta(\Gamma) = (X, E)$ is defined by

$$X = \Gamma \quad (4)$$

$$E = \{(x, x\delta) : x \in \Gamma, \delta \in \Delta\} \quad (5)$$

By this definition it will be natural to suppose that the coefficients of the evolution operator depends only on the generator used and not on the starting vertex, which can be interpreted as a homogeneity condition

$$W_{x\delta, x} = W_\delta. \quad (6)$$

In this case, the evolution operator may be written

$$W = \sum_{\delta \in \Delta} W_\delta U_\delta, \quad (7)$$

where $U_\delta = \sum_x |x\delta\rangle\langle x|$ is the unitary operator that right-multiplies each group element by δ . The unitarity equations (2-3) becomes

$$\sum_{\delta_1 \delta_2^{-1} = u} \overline{W}_{\delta_1} W_{\delta_2} = \delta_{u=e} \quad \forall \delta_1, \delta_2 \in \Delta, \quad (8)$$

where $\delta_{u=e} = 1$ if u equals the identity element e in the group Γ , and 0 otherwise.

For quantum walks over a Cayley graph, Proposition 1 implies a necessary condition over the elements of the generating set Δ :

Proposition 2. *Given a group Γ and a set Δ of elements generating Γ , a necessary condition for the existence of a scalar quantum walk of the form $W = \sum_{\delta \in \Delta} W_\delta U_\delta$ on the Cayley graph $C_\Delta(\Gamma)$ is that for all couples (δ_1, δ_2) of different elements of Δ , there exists at least one different couple (δ_3, δ_4) such that $\delta_1 \delta_2^{-1} = \delta_3 \delta_4^{-1}$.*

Proof. From Equation (8), we see that when the necessary condition is not satisfied, at least one of the coefficients W_i has to be zero. This is equivalent to modifying the graph (to removing the corresponding edges labeled with i). \square

In principle, it is impossible to solve the general problem of determining and classifying all groups obtained by the procedure of taking the quotient of a free group. This result is a consequence of the existence of finitely presented groups for which the word problem is unsolvable (see Theorem 7.2 in [10]). For this reason, it is probably hopeless to try solving the problem of determining and classifying all groups that verify the quadrangularity condition.

Here, we will instead consider groups with a small number of generators and build all possible minimal sets of relations verifying the quadrangularity condition. For the resulting groups, we will completely solve the system of equations (8) arising from the unitarity condition, and thus derive the most general evolution operator for a scalar quantum walk on the associated Cayley graphs. The general method to solve this problem is exposed in the next Section.

III. SOLVING THE UNITARITY CONDITION FOR THE EVOLUTION OPERATOR

Let us suppose we want to build a scalar quantum walk on a Cayley graph verifying the necessary condition from Proposition 2. When the homogeneity condition (6) is imposed, the number of variables describing the evolution operator decreases considerably since it is reduced to $d = |\Delta|$, the number of elements in the generating set Δ . The number of equations in the system (8) is also reduced, it is upper bounded by the number of different pairs of generators, that is, $\frac{d(d-1)}{2}$. Each equation in this system may be transformed into a bilinear equation

$$\mathbf{v}^\dagger P \mathbf{v} = 0, \quad (9)$$

$$\mathbf{v}^\dagger \mathbf{v} = 1, \quad (10)$$

where P is a $d \times d$ matrix with entries in $\{0, 1\}$ depending on the graph $C_\Delta(\Gamma)$ and $\mathbf{v} \in \mathbb{C}^d$ is a column vector having as components the elements W_i of the evolution operator. More precisely, if we define as

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, \mathbf{e}_d = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \quad (11)$$

the vectors in the standard basis of \mathbb{C}^d , we have $\mathbf{v} = \sum_{i=1}^d W_i \mathbf{e}_i$. Let $\{\lambda_1, \dots, \lambda_d\}$ be the d eigenvalues of P (with algebraic multiplicities). If the geometric multiplicities of these eigenvalues equal their algebraic multiplicities, we may build an orthonormal basis $\{\mathbf{v}_1, \dots, \mathbf{v}_d\}$ out of eigenvectors of P . Developing \mathbf{v} in this basis, we may write $\mathbf{v} = \sum_{j=1}^d \alpha_j \mathbf{v}_j$ so that Equation (9) becomes

$$\sum_{j=1}^d \lambda_j |\alpha_j|^2 = 0, \quad (12)$$

whereas the normalization equation (10) is simply

$$\sum_{j=1}^d |\alpha_j|^2 = 1. \quad (13)$$

The relation between the new coefficients α_j and the evolution operator coefficients W_i is then given by

$$W_i = \sum_j \alpha_j \mathbf{e}_i^\dagger \mathbf{v}_j. \quad (14)$$

In the next section, we will use this approach to build scalar quantum walks on groups with few generators, or prove that no such walk exists.

IV. APPLICATION

Let us consider groups denoted as $\Gamma = \langle \Delta | R \rangle$, using the standard free group representation where Δ is a set of generators for the group Γ and R is a set of relations among these generators, and determine whether the associated Cayley graph admits a scalar quantum walk.

A. Groups finitely presented with two generators

The simplest case is a group finitely generated with two generators. We denote the set of generators as $\Delta = \{x, y\}$. There are only two possible couples (x, y) and (y, x) and therefore the only relation which makes the necessary condition satisfied is $xy^{-1} = yx^{-1}$. Let us consider the corresponding group $\Gamma = \langle x, y | xy^{-1} = yx^{-1} \rangle$, and check whether there is a scalar quantum walk on the associated Cayley graph $C_\Delta(\Gamma)$. The unitarity equations (8) become

$$\begin{cases} \overline{W}_x W_y + \overline{W}_y W_x = 0 \\ \overline{W}_x W_x + \overline{W}_y W_y = 1, \end{cases} \quad (15)$$

which can be written as bilinear equations (9-10) with $\mathbf{v} = \begin{pmatrix} W_x \\ W_y \end{pmatrix}$ and $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Developing \mathbf{v} in the basis formed by the eigenvectors of P , that is $\mathbf{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\mathbf{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, with respective eigenvalues $\lambda_1 = 1$ and $\lambda_2 = -1$, we see that Equations (12-13) become

$$\begin{cases} |\alpha_1|^2 - |\alpha_2|^2 = 0 \\ |\alpha_1|^2 + |\alpha_2|^2 = 1, \end{cases} \quad (16)$$

so that the solution is up to a global phase

$$\begin{cases} W_x = \cos \phi \\ W_y = i \sin \phi \end{cases} \quad (17)$$

for $\phi \in [0, 2\pi]$. Thus, there exists a scalar quantum walk on the Cayley graph $C_\Delta(\Gamma)$ for the group considered here.

Interestingly, this is also true for all groups finitely presented with two generators satisfying $xy^{-1} = yx^{-1}$, since adding other types of relation will not modify the system of equations (8). In particular, we can add some relations to the previous infinite group in order to make it finite. Hence, we show that there is a scalar quantum walk for the dihedral group $D_n = \langle x, y | x^n = e, y^2 = e, (xy)^2 = e \rangle$, with generating set $\Delta = \{x, y\}$. The evolution operator coefficients are also given by Eqs. (17), and the corresponding Cayley graph is both strongly quadrangular and specular (it was first presented in [5]).

Finally, let us note that the hypercube of dimension 2 can be obtained as the Cayley graph of the $n = 2$ case of D_n , that is, $D_2 = \langle x, y | x^2 = e, y^2 = e, xy = yx \rangle$, with $\Delta = \{x, y\}$. We conclude that the hypercube of dimension 2 therefore also accepts a scalar quantum walk.

B. Groups finitely presented with three generators

In the case of three generators there are six possible couples, and then a large number of groups, in principle 6^5 . We will use the following representation in order to simplify the counting of the possibles graphs verifying the necessary condition. We associate each pair of generators (δ_i, δ_j) to the vertex element $M_{i,j}$ of a 3×3 grid M (see Fig. 1). A relation $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ may then be represented as an edge between vertices (δ_i, δ_j) and (δ_k, δ_l) .

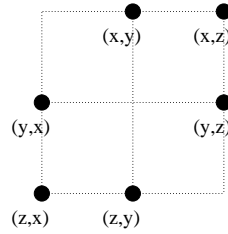


FIG. 1: Representation of the relations between generators as a grid. A relation $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ will be represented as an edge between vertices (δ_i, δ_j) and (δ_k, δ_l) .

From the necessary condition, we know that the grids corresponding to a valid graph are those where all vertices are connected with at least another vertex. Note that there is no element in the diagonal, since there are no couples of the form (δ_i, δ_i) . Moreover, the different edges are not independent, since $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ is equivalent to $\delta_j \delta_i^{-1} = \delta_l \delta_k^{-1}$ (this implies a symmetry with respect to the diagonal axis), while by transitivity the relations $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ and $\delta_k \delta_l^{-1} = \delta_m \delta_n^{-1}$ imply $\delta_i \delta_j^{-1} = \delta_m \delta_n^{-1}$. We also see that not all edges are interesting since a vertical or an horizontal edge implies a relation of the form $\delta_i = \delta_j$ and thus a trivial reduction of the number of generators.

By a straightforward (but tedious) inspection of all grids, it can be shown that among the 6^5 groups finitely presented with three generators, there are only three non-equivalent groups (without trivial reduction) that satisfy the necessary condition (see Fig. 2). There remains to check whether there actually exists a scalar quantum walk on the Cayley graph built from these three groups:

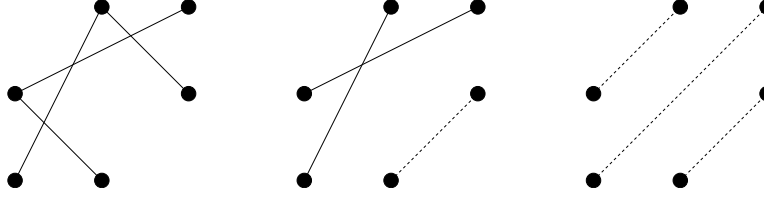


FIG. 2: Representation of the three sets of relations implying no reduction. Valid sets of relations are those for which any vertex is connected to at least one other vertex. Other sets of relations either reduce to one of the three sets represented here (possibly up to a permutation of the generators) or imply a reduction of the number of generators.

- i) $\Gamma = \langle x, y, z | xy^{-1} = yz^{-1}, xy^{-1} = zx^{-1} \rangle$ and $\Delta = \{x, y, z\}$

Note that the group Γ may equivalently be written as $\langle x, y, z | z = xy^{-1}x, (xy^{-1})^3 = e \rangle$. The unitarity condition equations (2-3) become

$$\begin{cases} \overline{W}_x W_y + \overline{W}_z W_x + \overline{W}_y W_z = 0 \\ \overline{W}_x W_x + \overline{W}_y W_y + \overline{W}_z W_z = 1, \end{cases} \quad (18)$$

which can be written as a bilinear hermitian form with $\mathbf{v} = \begin{pmatrix} W_x \\ W_y \\ W_z \end{pmatrix}$ and $P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$. Using the expansion of \mathbf{v} in terms of the eigenvectors of P , the system reduces to

$$\begin{cases} |\alpha_1|^2 + e^{i\frac{2\pi}{3}} |\alpha_2|^2 + e^{-i\frac{2\pi}{3}} |\alpha_3|^2 = 0 \\ |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 = 1, \end{cases} \quad (19)$$

so that the solution is (up to a global phase)

$$\begin{cases} W_x = \frac{1}{3}(1 + e^{i\phi_1} + e^{i\phi_2}) \\ W_y = \frac{1}{3}(1 + e^{i\frac{2\pi}{3}} e^{i\phi_1} + e^{-i\frac{2\pi}{3}} e^{i\phi_2}) \\ W_z = \frac{1}{3}(1 + e^{-i\frac{2\pi}{3}} e^{i\phi_1} + e^{i\frac{2\pi}{3}} e^{i\phi_2}). \end{cases} \quad (20)$$

- ii) $\Gamma = \langle x, y, z | xy^{-1} = zx^{-1}, yz^{-1} = zy^{-1} \rangle$ and $\Delta = \{x, y, z\}$

Using a similar method, we find the following general solution:

$$\begin{cases} W_x = \cos \phi \\ W_y = \frac{1+i(-1)^q}{2} \sin \phi \\ W_z = -\frac{1-i(-1)^q}{2} \sin \phi, \end{cases} \quad (21)$$

for $\phi \in [0, 2\pi]$ and q any integer.

- iii) $\Gamma = \langle x, y, z | xy^{-1} = yx^{-1}, xz^{-1} = zx^{-1}, yz^{-1} = zy^{-1} \rangle$ and $\Delta = \{x, y, z\}$

We obtain that there is no solution (the proof is also based on the same method as above).

If we add more relations of the type $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ to these groups, reductions appear and we end up with one of the following groups with less than three generators (see Fig. 3):

- iv) $\Gamma = \langle x, y | xy^{-1} = yx^{-1} \rangle$ and $\Delta = \{x, y\}$

This group with two generators has been presented in Section IV A and admits a scalar quantum walk.

- v) $\Gamma = \langle x \rangle$ and $\Delta = \{x\}$

The free group with one generator admits a trivial scalar quantum walk, which acts as a shift operator on an infinite line. Adding a relation $x^n = e$, we obtain the cyclic group $C_n = \langle x | x^n = e \rangle$, and the associated Cayley graph becomes a cycle, which thus also accepts such a trivial scalar quantum walk.

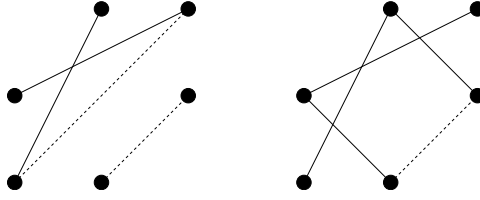


FIG. 3: Representation of the two sets of relations implying reductions of the number of generators. In the first case, we obtain $x = y$, while in the second, we have $x = y = z$. Note that other sets of relations may reduce to these cases, possibly up to some permutation of the generators.

Of course, there exist other relations beyond these of the type $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$, so that we may build further groups by adding other relations. Nonetheless, as long as these additional relations do not imply relations of the previous type nor trivial reductions, they will have no influence on the possible existence of a scalar quantum walk on the associated Cayley graphs.

For instance, adding relations $x^2 = e$ and $y^2 = e$ to the above group (i), we obtain the symmetric group $S_3 = \langle x, y | x^2 = e, y^2 = e, (xy)^3 = e \rangle$ with two generators. This is the group of permutations of three elements, x corresponding to a permutation of the first two elements, y to a permutation of the last two elements, and xyx to a permutation of the first and third elements. Taking $\Delta = \{x, y, xyx\}$, the corresponding Cayley graph therefore admits a scalar quantum walk, with evolution operator coefficients given by Eq. (20).

Similarly, if we add the relation $y^2 = x$ to the group (ii), the set of relations imply $y^3 = z$ and $y^4 = e$, so that we obtain the cyclic graph $C_4 = \langle y | y^4 = e \rangle$. Since we use as generators all the group elements except the identity e , that is, $\Delta = \{y, y^2, y^3\}$, the Cayley graph reduces to the complete graph over four vertices, which thus admits a scalar quantum walk with evolution operator coefficients given by Eq. (21).

Finally, if we impose the additional relations $x^2 = y^2 = z^2 = e$ to the group (iii) without reduction, the associated Cayley graph becomes the hypercube in dimension 3. It follows that even though there exists a scalar quantum walk on the hypercube in dimension 2, as we have seen above, there is no such walk in dimension 3.

C. Other examples

vi) Cayley graphs of the cyclic group $C_n = \langle a | a^n = e \rangle$.

We have already found a way to define a scalar quantum walk on a cycle, which is the simplest Cayley graph of the cyclic group C_n . Here, we show how to build homogeneous scalar quantum walk on more general Cayley graphs of the cyclic group (see also [11]). The elements of C_n may be written as $\{a^i | i = 0, \dots, n\}$. The necessary condition implies that if a^i and a^j are taken as generators to build the Cayley graph, we must also take some elements a^k and a^l such that $(i - j) - (k - l) \bmod n = 0$.

In particular, if n is a multiple of d , this condition is satisfied if the generator set, with d elements, is taken as $\Delta = \{a^{j\frac{n}{d}+l} | j = 0, \dots, d-1\}$, where l is some integer. The unitarity condition equations (2-3) become

$$\sum_{j=0}^{d-1} \overline{W}_j W_{(j+i) \bmod n} = \delta_{i,0} \quad (22)$$

for $i = 0, \dots, d-1$ and the solution is

$$W_j = \frac{1}{d} \sum_{k=0}^{d-1} e^{i\theta_k} e^{i\frac{2\pi kj}{d}}. \quad (23)$$

Hence, there are $d-1$ real parameters that define the evolution operator for this family of Cayley graphs of the cyclic groups. This is not exhaustive for cyclic groups and there are also scalar quantum walks on Cayley graphs outside this family, we have already seen one example, the complete graph over 4 vertices, and another example will be given below, in the context of Johnson graphs.

The $d = n$ special case corresponds to the complete graph with self-loops (the self-loops come from the fact that we also take as generator the identity e , which maps any group element to itself). This graph trivially accepts scalar quantum walks since any unitary matrix without zero entries may be taken as a diffusion operator

(note that here we give the general form of *homogeneous* scalar quantum walks). In particular, taking $\theta_0 = \pi$ and $\theta_k = 0$ for all $k \neq 0$ yields the usual diffusion operator from Grover's algorithm, with $W_0 = 1 - 2/n$ and $W_k = -2/n$ for all $k \neq 0$. The $d = 1$ special case reduces to the cycle, that we have already seen above in the context of the free group with one generator.

vii) The Johnson graphs $J(n, k)$.

The Johnson graph $J(n, k)$ is defined as the graph having as vertices the C_n^k subsets of size k of a set of n elements, and such that two subsets are linked by an edge if they have $k - 1$ elements in common. Let us note that $J(n, n - k) = J(n, k)$.

All Johnson graphs verify the quadrangularity condition. Numerically, we have obtained that the Johnson graphs $J(n, k)$ for small values of n and k also verify the strong quadrangular condition. Whether they admit a scalar quantum walk in general is an open question. However, our method may help to solve this problem on a case by case basis. Indeed, while until now we have built Cayley graphs from groups, we may take the opposite point of view and try to build a group that accepts a given graph as Cayley graph. For instance, the graph $J(4, 2)$ can be described as a Cayley graph of the cyclic group of order six $C_6 = \langle \delta_1 | \delta_1^6 = e \rangle$. Defining $\delta_2 = \delta_1^2$, the Cayley graph, represented in Fig. 4, is then constructed with the generating set $\Delta = \{\delta_1, \delta_1^{-1}, \delta_2, \delta_2^{-1}\}$. The equations are thus

$$\begin{cases} \overline{W}_{\delta_2} W_{\delta_1^{-1}} + \overline{W}_{\delta_2^{-1}} W_{\delta_1} + \overline{W}_{\delta_1} W_{\delta_2^{-1}} + \overline{W}_{\delta_1^{-1}} W_{\delta_2} = 0 \\ \overline{W}_{\delta_2} W_{\delta_1} + \overline{W}_{\delta_1^{-1}} W_{\delta_2^{-1}} = 0 \\ \overline{W}_{\delta_1} W_{\delta_1^{-1}} + \overline{W}_{\delta_2^{-1}} W_{\delta_2} = 0 \\ \overline{W}_{\delta_1} W_{\delta_1} + \overline{W}_{\delta_1^{-1}} W_{\delta_1^{-1}} + \overline{W}_{\delta_2} W_{\delta_2} + \overline{W}_{\delta_2^{-1}} W_{\delta_2^{-1}} = 1. \end{cases} \quad (24)$$

Using the previous method, we show that the general solution is

$$\begin{cases} W_{\delta_1} = \frac{1}{2} e^{i\phi} \\ W_{\delta_1^{-1}} = \frac{1}{2} \\ W_{\delta_2} = \frac{(-1)^q}{2} \\ W_{\delta_2^{-1}} = \frac{(-1)^{q+1}}{2} e^{i\phi} \end{cases} \quad (25)$$

for $\phi \in [0, 2\pi]$ and q any integer.

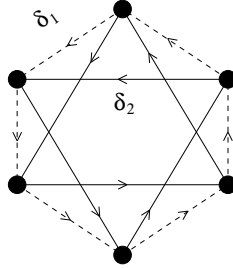


FIG. 4: Johnson graph $J(4, 2)$, which may be seen as the Cayley graph of the cyclic group $C_6 = \langle \delta_1 | \delta_1^6 = e \rangle$ with generating set $\Delta = \{\delta_1, \delta_1^{-1}, \delta_2, \delta_2^{-1}\}$, where $\delta_2 = \delta_1^2$. Note that we have only represented the oriented edges corresponding to δ_1 and δ_2 , and not their inverses, corresponding to δ_1^{-1} and δ_2^{-1} .

Going beyond $J(4, 2)$, we have also tested numerically whether Johnson graphs verify the strong quadrangularity condition. We have obtained that, at least within a computationally achievable range of values n and k , they always verify the strong quadrangularity condition, except for the pathological case $J(3, 1)$ (and consequently $J(3, 2)$) which corresponds to the complete graph over three vertices (without self-loops) and does obviously not admit a scalar quantum walk. Consequently, it may be the case that, in addition to the special case $J(4, 2)$, most Johnson graphs with large n and k admit a scalar quantum walk.

V. CONCLUSION

We have obtained a simple necessary condition for the existence of a scalar quantum walk on Cayley graphs, as well as a general method to construct its evolution operator (or to conclude that no such walk exists) when the necessary

condition is fulfilled. Even if the homogeneity of the evolution operator is required, scalar quantum walks often exist on Cayley graphs, and we have presented a series of examples for finitely presented groups (see Table I).

Generators Δ	Relations R	Existence of homogeneous SQW	Groups or graphs
x	\emptyset	yes	Cycle graphs
x, y	$xy^{-1} = yx^{-1}$	yes	Dihedral groups D_n , Hypercube in dim. 2
x, y, z	$xy^{-1} = yz^{-1} = zx^{-1}$	yes	Symmetric group S_3
x, y, z	$xy^{-1} = zx^{-1}, yz^{-1} = zy^{-1}$	yes	Complete graph over 4 vertices
x, y, z	$xy^{-1} = yx^{-1}, xz^{-1} = zx^{-1}, yz^{-1} = zy^{-1}$	no	Hypercube in dim. 3
$a^{j\frac{d}{2}+k}$ ($j = 0, \dots, d-1$)	$a^n = e$	yes	Complete graph with self-loops, Cycle graphs
a, a^{-1}, a^2, a^{-2}	$a^6 = e$	yes	Johnson graph $J(4, 2)$

TABLE I: Summary of our results. The first two columns define the groups by giving their free group representation $\Gamma = \langle \Delta | R \rangle$, where Δ is the set of generators and R is the set of relations between these generators. The third column specifies whether there exists a homogeneous scalar quantum walk (SQW) on the associated Cayley graph. The last column lists groups or graphs also concerned by this result.

We have unfortunately not been able to answer completely the open question of deriving a general necessary and sufficient condition for the existence of a quantum operator on a graph. We have shown, however, that assuming homogeneity significantly simplifies the problem and allows to solve it explicitly for a large class of Cayley graphs. For non Cayley graphs, there is no general procedure to assign equal coefficients to different edges in a non-arbitrary way. However, non-homogeneous quantum walks may also be used to construct quantum algorithms, so that exploring which general graphs admit scalar quantum walks certainly deserves further investigation.

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